

Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

March 10, 2013

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World-Class Columbia System Being Retired After Nearly 9 Years of Supporting Users



- In February, 3 of the 4 remaining Columbia supercomputer nodes were retired.
- During nearly 9 years of service, Columbia provided over 3 billion CPU-hours to users from all of NASA's Mission Directorates.
- Born of a unique partnership with industry (SGI, Intel, and Voltaire), Columbia went from concept to operation in only 120 days.
- Beginning in July 2004, as each node arrived, it
 was put into production—providing an immediate
 increase to NASA's computational resources—and
 by completion, a factor of 10 increase.
- Named to honor the crew of the shuttle Columbia, the system enabled debris trajectories as well as entry, descent, and landing analyses that were crucial for returning the space shuttle to flight.
- One Columbia node remains while users complete their migration to Pleiades or Endeavour.

Mission Impact: Access to world-class computing systems provides NASA mission directorates with cutting-edge tools to accomplish their goals and objectives.



The original Columbia supercomputer was comprised of twenty 512-processor SGI Altix 3700 and 3700-BX2 nodes. The system had 10,240 Intel Itanium 2 processors and 20 terabytes of memory. Four nodes were configured so that 2,048 processors could be used with a single, shared memory).

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Endeavour Supercomputer Now Available to Users for Production Work



- On February 22, the HECC Supercomputing Systems team released the new Endeavour supercomputer to users for production work; Endeavour replaces the Columbia system, installed in 2004.
- Endeavour is an SGI Ultra Violet (UV) system comprising two UV 2000 nodes with Intel E5-4650L (Sandy Bridge) processors, featuring:
 - One 1,024-core node with 4 terabytes (TB) of memory;
 - One 512-core node with 2 TB of memory;
 - Direct access to the Pleiades scratch filesystem simplifies data sharing between jobs on Pleiades and Endeavour.
- Endeavour provides users with the same sharedmemory capabilities that Columbia provided, allowing a single process to access all memory on the node, but has better processor performance with the new Sandy Bridge processors.
- For more details, see the Endeavour resource page: <u>http://www.nas.nasa.gov/hecc/resources/</u> <u>endeavour.html</u>

Mission Impact: The Endeavour supercomputer will provide NASA users with a unique, shared-memory capability necessary to advance mission priorities.



The Endeavour supercomputer provides more high-end computing resources for users while occupying just 10% of Columbia's footprint.

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HECC Experts Prototype Cloud Bursting Capability



- HECC's Application Performance and Productivity (APP) team is evaluating the use of cloud computing environments for providing extra resources to handle surges in computing demand by NASA users that cannot be met by existing HECC resources.
- As part of the evaluation, the APP team successfully prototyped a methodology to "burst" a job from a Portable Batch System (PBS) scheduling queue on Pleiades to both an external cloud (Amazon EC2) and an internal private cloud.
- The team implemented steps needed for this test, including:
 - Setting up the execution environment on the cloud;
 - Staging input files and the executable;
 - Starting and monitoring the execution;
 - Returning the output to Pleiades at the end of the execution;
 - Disassembling the execution environment.
- The team is continuing to resolve security-related issues with transferring data in and out of the secure HECC enclave; and handle errors and faults in the cloud computing environment.

Mission Impact: Analyses of the effectiveness of transferring jobs from HECC resources to run in cloud environments could help handle surges in demand and improve turnaround time for NASA users.



The internal cloud testbed, an SGI rack comprising 16 dual-socket Intel Xeon Sandy Bridge nodes each with 64 gigabytes of main memory and 4 terabytes of local disk storage.

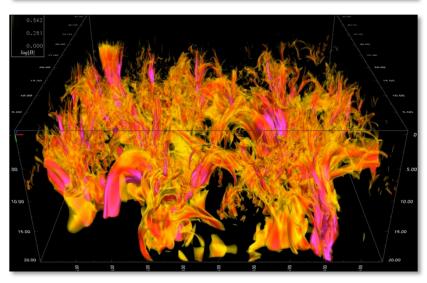
POCs: Steve Heistand, steve.heistand@nasa.gov, (650) 604-4369, NASA Advanced Supercomputing Division, Computer Sciences Corp.; Piyush Mehrotra, piyush.mehrotra@nasa.gov, (650) 604-5126; NASA Advanced Supercomputing Division

Pleiades Enables High-Fidelity Modeling and Simulation of Solar Weather



- Researchers at Michigan State University (MSU) are modeling the Sun's weather to study the magnetic fields on the solar surface that control heating of the solar chromosphere and corona and eruption of flares and coronal mass ejections.
- Enabled by Pleiades, the MSU team obtains numerical solutions to the conservation equations for mass, momentum, and energy plus the induction equation for the magnetic field.
- A key result is that inverting observations of small-scale, weak magnetic fields (less than 100-200 Gauss) is unreliable, due to the complex vertical and horizontal structure of the magnetic and velocity fields, and is exacerbated by the limited resolution of telescopes.
- Results are being used to evaluate the ability of Inversions of Stokes profiles to obtain accurate 3D magnetic fields, in order to understand and evaluate data from NASA missions such as the Solar Dynamics Observatory and Hinode.
- These high-fidelity simulations require several million processor hours on Pleiades, without which they would be would be impossible to produce.

Mission Impact: The Pleiades supercomputer is critical to producing high-fidelity solar simulations used to understand and evaluate data from NASA missions such as the Solar Dynamics Observatory and Hinode.



Complex magnetic loop structure produced by magnetoconvection. Tim Sandstrom, NASA/Ames

POC: Robert Stein, stein@pa.msu.edu, (517) 884-5613, Michigan State University

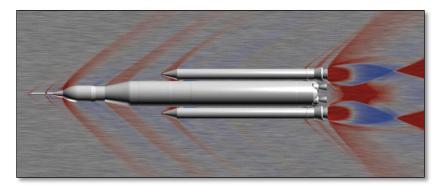
^{*} HECC provided supercomputing resources and services in support of this work.

HECC Resources Continue Critical Support for Modeling & Simulation of Space Launch System



- Researchers in the NASA Advanced Supercomputing Division are performing computational fluid dynamics (CFD) simulations to support the design of NASA's next-generation Space Launch System (SLS).
- Candidate SLS designs are simulated at select points over the ascent trajectory and at multiple angles of attack, producing comprehensive aerodynamic databases.
- These results provide input data for trajectory and structural analyses that are used to improve the vehicle's design.
- CFD simulations aided critical decisions early in the design cycle before wind tunnel data was available; ongoing simulations impact the design of vehicle's shape, internal structural components, layout of the core stage fairing and main engines, booster separation analysis, and venting methods.
- The Pleiades supercomputer enables the team to quickly and efficiently produce aerodynamic databases that require hundreds of large scale simulations, using 300 cores and 40 hours of wallclock time per simulation.

Mission Impact: Enabled by HECC supercomputing resources, CFD simulations support critical design decisions for the agency's next-generation Space Launch System, using efficient and cost-effective methods that provide design engineers with timely inputs to meet SLS development milestones.



Power-on simulations of the Space Launch System (SLS) were performed to analyze the vehicle's aerodynamic features. The figure shows contours of pressure and streamlines that indicate the velocity flow patterns, and plumes that display the shock structures generated by the solid rocket booster jets. Simulations such as these support SLS engineers making critical vehicle design decisions. *Jeffrey Housman, Cetin Kiris, NASA/Ames*

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HECC Facility Hosts Several Visitors and Tours in February 2013



- HECC hosted 5 tour groups in February; guests learned about the agency-wide missions being supported by Pleiades, and viewed scientific results on the hyperwall-2 system. Visitors this month included:
 - A group of attendees from the Living With a Star (LWS)
 Workshop 2013 met with HECC visualization experts,
 utilizing the hyperwall-2 system for Solar Dynamic
 Observatory research discussions;
 - A group from the Fermi Gamma-ray Space Telescope project at the SLAC National Accelerator Laboratory met with visualization lead Chris Henze regarding possible future collaborations;
 - A large group of teachers from East Side Union High School District received an overview of the NASA Advanced Supercomputing (NAS) facility, with a hyperwall-2 demonstration and computer room tour;
 - NASA Ames Space Biosciences Division Chief Sid Sun accompanied guests from the Russian Academy Of Sciences Institute Of Biomedical Problems during an overview of the NAS facility, including a hyperwall-2 demo and tour of the computer room.



Thirty-two teachers from the East Side Union High School District, San Jose, CA, visited the NASA Advanced Supercomputing facility as part of their science, technology, engineering and math (STEM) service at NASA Ames.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputer Division

Papers and Presentations



- "Global Data Sets of Vegetation Leaf Area Index (LAI)3g and Fraction of Photosynthetically Active Radiation (FPAR)3g Derived from Global Inventory Modeling and Mapping Studies (GIMMS) Normalized Difference Vegetation Index (NDVI3g) for the Period 1981 to 2011," Z. Zhu, J. Bi, R. Nemani, et al., Remote Sensing, vol. 5, issue 2, February 22, 2013. * http://www.mdpi.com/2072-4292/5/2/927
- "Validity of Hydrostatic Equilibrium in Galaxy Clusters from Cosmological Hydrodynamical Simulations," D. Suto, H. Kawahara, T. Kitayama, S. Sasaki, Y. Suto, R. Cen, arXiv:1302.5172 [astro-ph.CO], February 421. * http://arxiv.org/abs/1302.5172
- "Permeation of Aldopentoses and Nucleosides Through Fatty Acid and Phospholipid Membranes: Implications to the Origins of Life," C. Wei, A. Porhorille, Astrobiology, vol. 13, issue 2, pp. 177-188, February 19, 2013. *
 http://online.liebertpub.com/doi/full/10.1089/ast.2012.0901
- "Numerical Simulations of Radiatively-Driven Dusty Winds," M. R. Krumholz, T. A. Thompson, arXiv:1302.4440 [astro-ph.CO], February 18, 2013. * http://online.liebertpub.com/doi/full/10.1089/ast.2012.0901

^{*} HECC provided supercomputing resources and services in support of this work.

Papers and Presentations



- "Aerodynamics and Debris Transport for the Space Shuttle Launch Vehicle,"
 S. Rogers, AIAA SF Dinner Meeting, Michael's at Shoreline, Mountain View, California, February 13, 2013. *
 http://www.aiaa-sf.org/dmtg13/02.html
- "Approach to Integrate Global-Sun Models of Magnetic Flux Emergence and Transport for Space Weather Studies," N. Mansour, LWS Workshop 2013, February 11-15, 2013, NASA Ames Research Center. * http://ntrs.nasa.gov/search.jsp?R=20130008684
- "Absorption Efficiencies of Forsterite. I: DDA Explorations in Grain Shape and Size,"
 S. S. Lindsay, D. H. Wooden, et al., arXiv:1302.0788 [astro-ph.EP], February 4, 2013. *
 http://arxiv.org/abs/1302.0788
- "The Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP):
 Overview and Description of Models, Simulations and Climate Diagnostics,"
 J.-F. Lamarque, et al., Geoscientific Model Development, vol. 6, pp. 179-206,
 February 2013. *

http://www.geosci-model-dev.net/6/179/2013/gmd-6-179-2013.pdf

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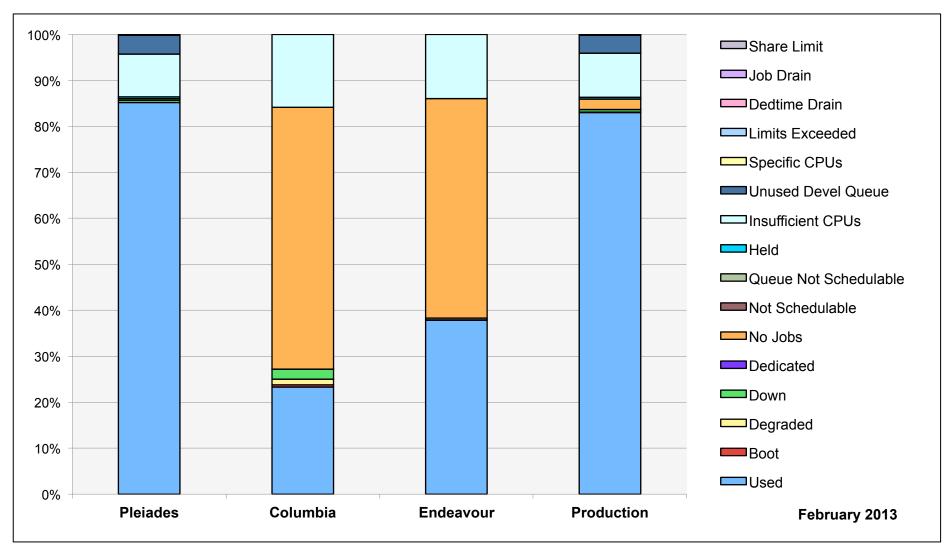
News and Events



Journey to the Limits of Spacetime, Texas Advanced Computing Center Press Release,
The University of Texas at Austin, February 13, 2013 – Using 3D simulations created on
supercomputers at the NASA Advanced Supercomputing Division, the Texas Advanced
Computing Center, and the National Institute for Computational Sciences, researchers are
now able to visualize the forces around black holes with much greater detail.
http://www.tacc.utexas.edu/news/feature-stories/2012/journey-to-the-limits-of-spacetime

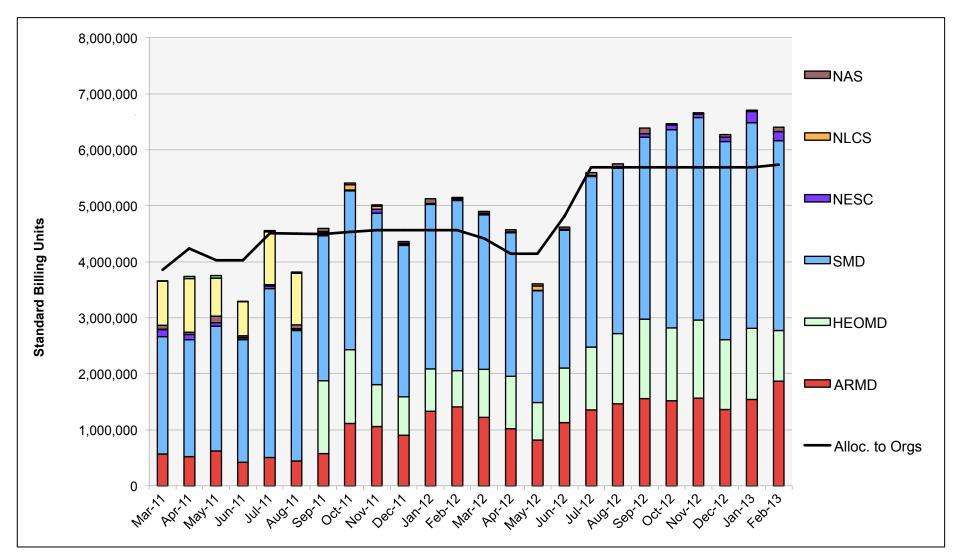
HECC Utilization





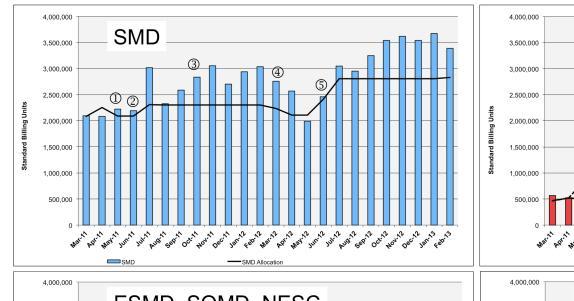
HECC Utilization Normalized to 30-Day Month

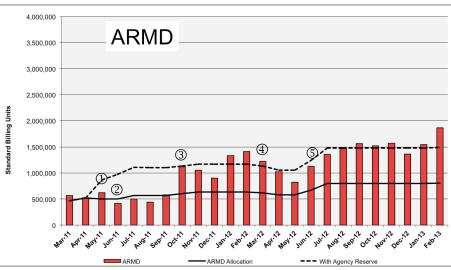


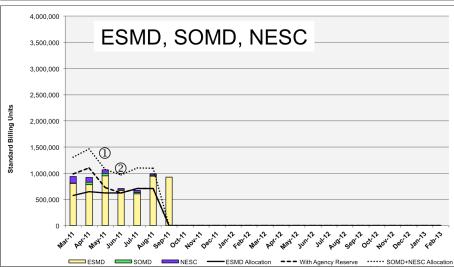


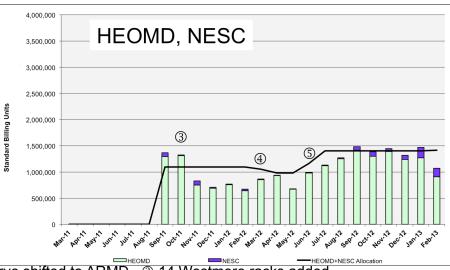
HECC Utilization Normalized to 30-Day Month









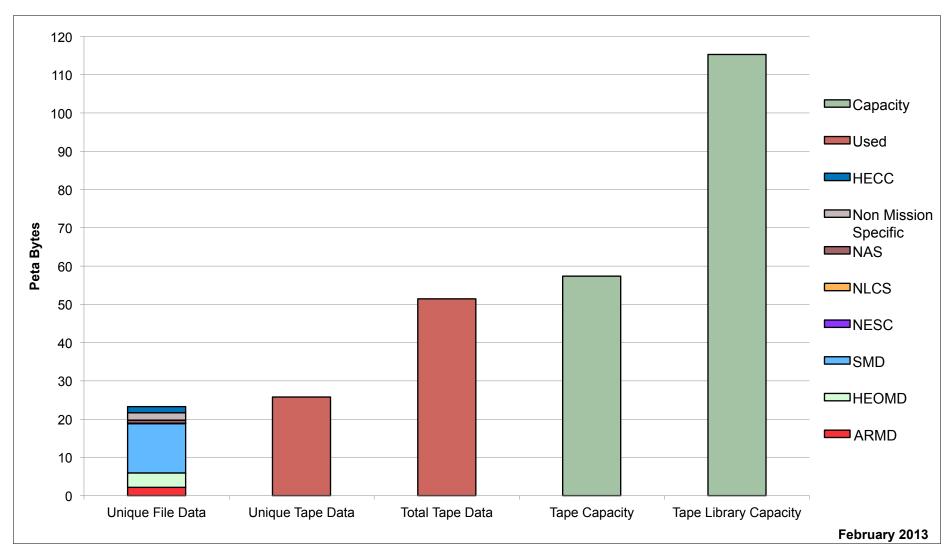


① Allocation to orgs. decreased to 75%, Agency reserve shifted to ARMD ② 14 Westmere racks added

③ 2 ARMD Westmere racks added ④ 28 Harpertown racks removed ⑤ 24 Sandy Bridge racks added

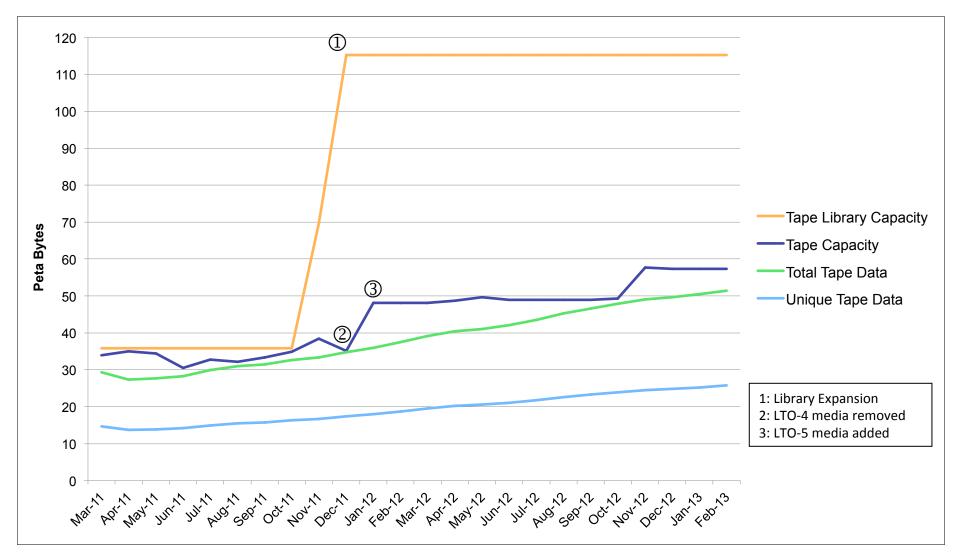
Tape Archive Status





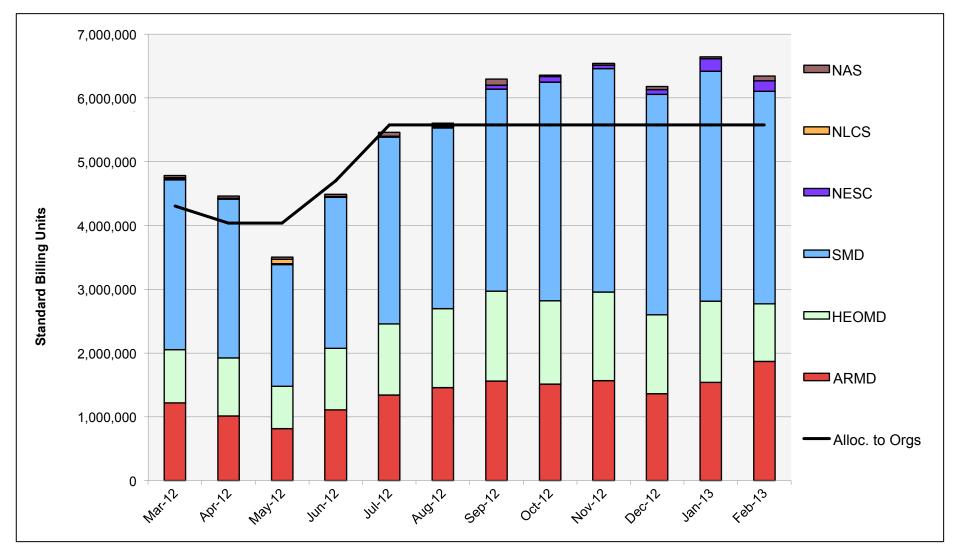
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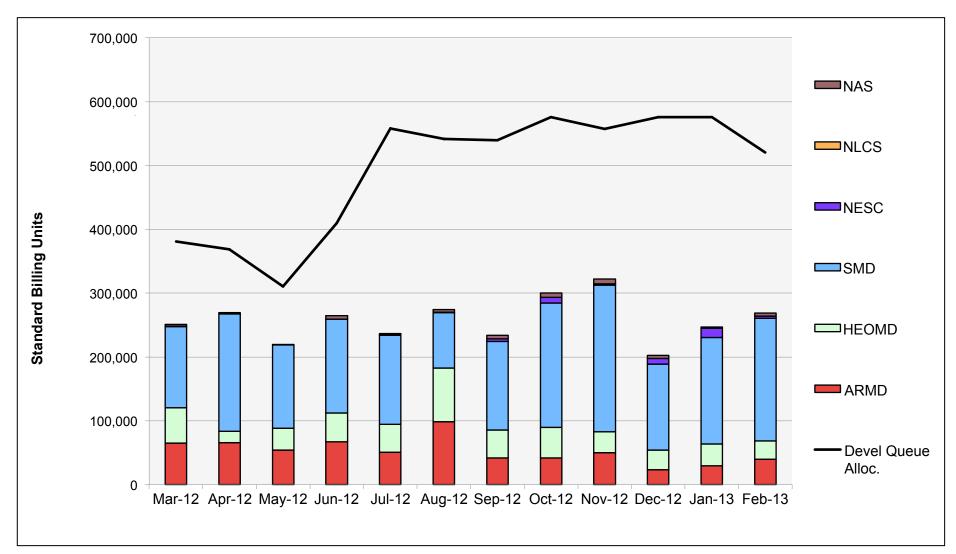
Pleiades: SBUs Reported, Normalized to 30-Day Month





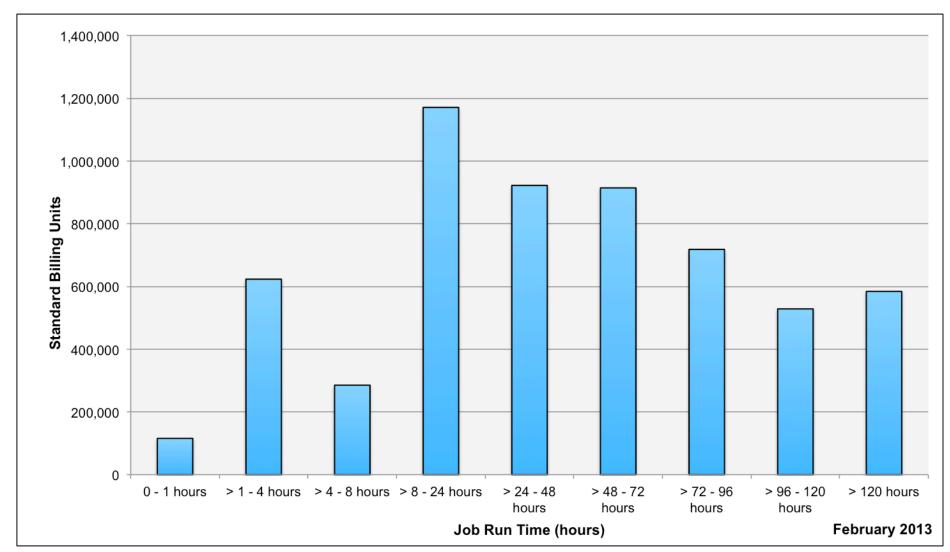
Pleiades: Devel Queue Utilization





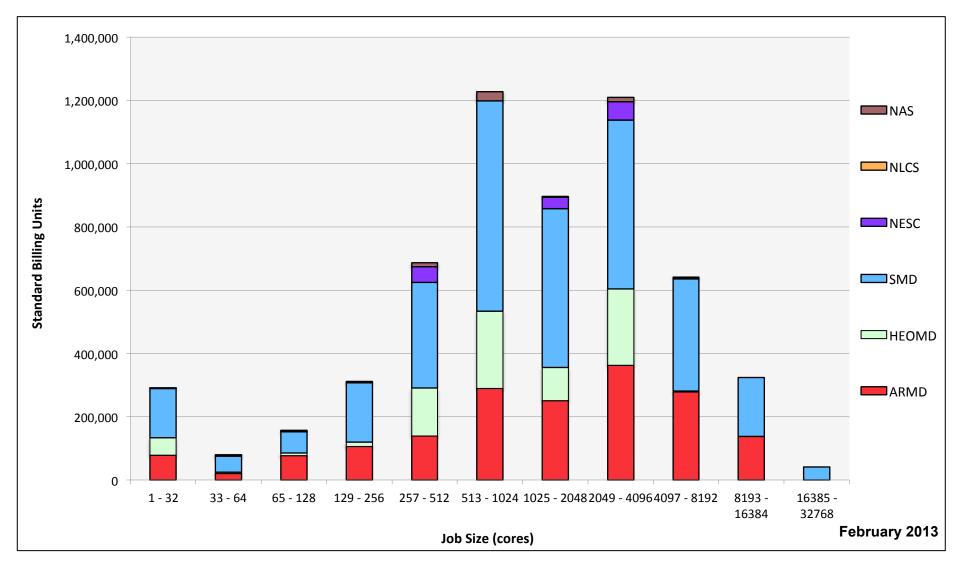
Pleiades: SBUs Reported, Normalized to 30-Day Month





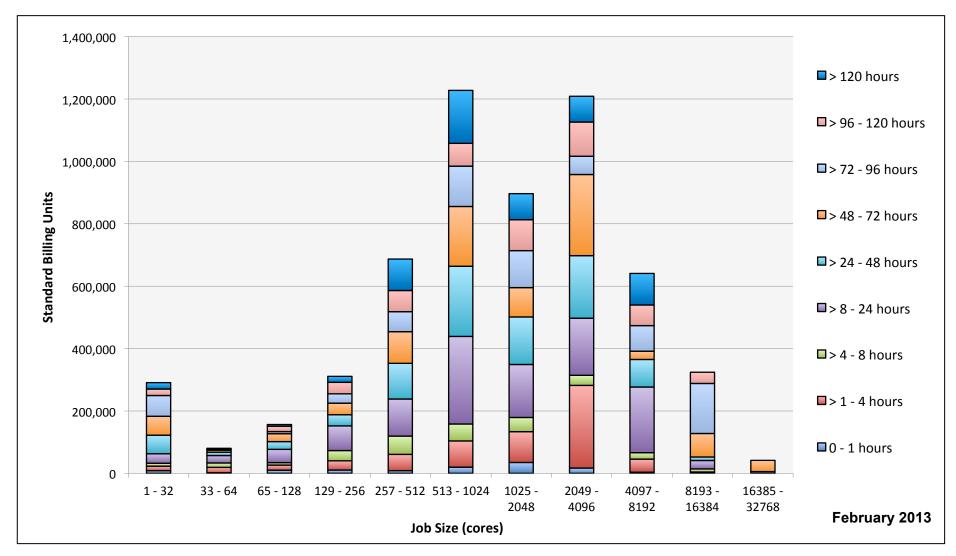
Pleiades: Monthly Utilization by Size and Mission





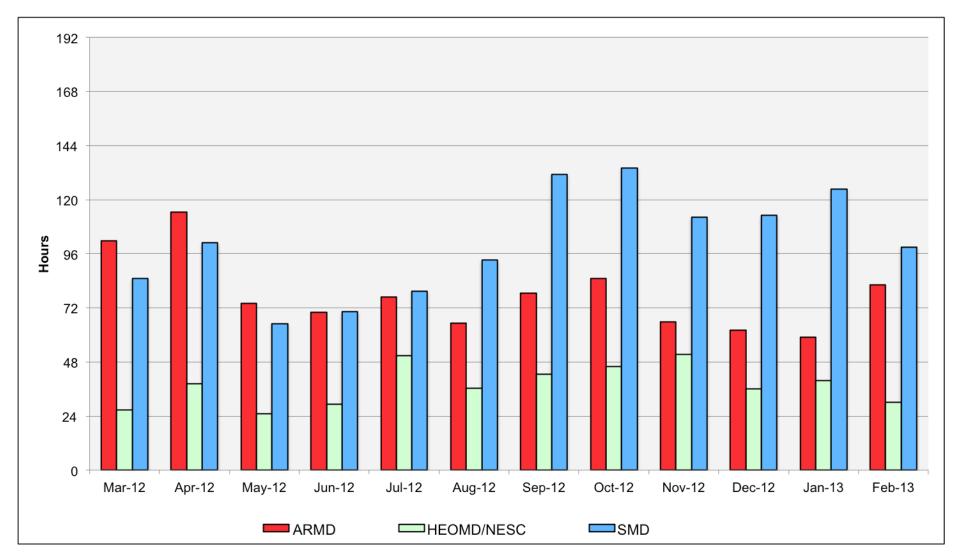
Pleiades: Monthly Utilization by Size and Length





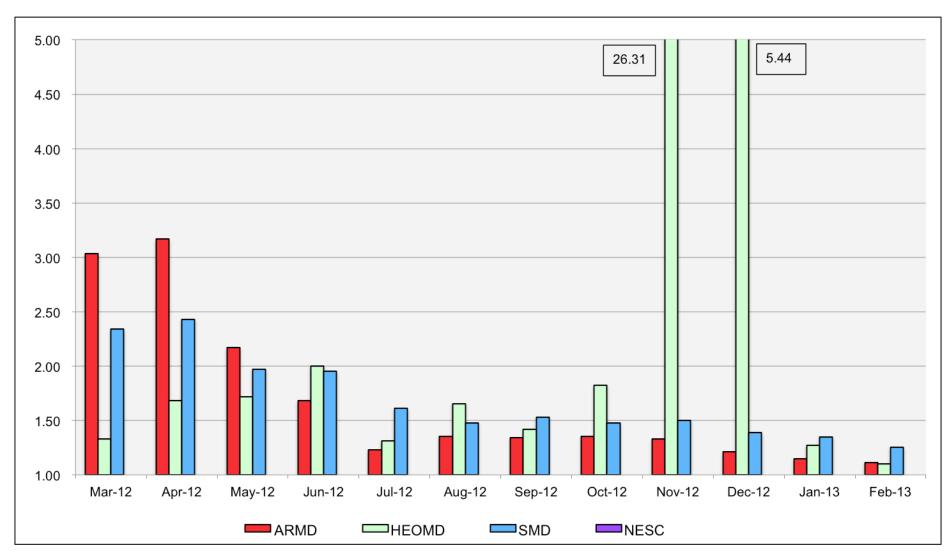
Pleiades: Average Time to Clear All Jobs





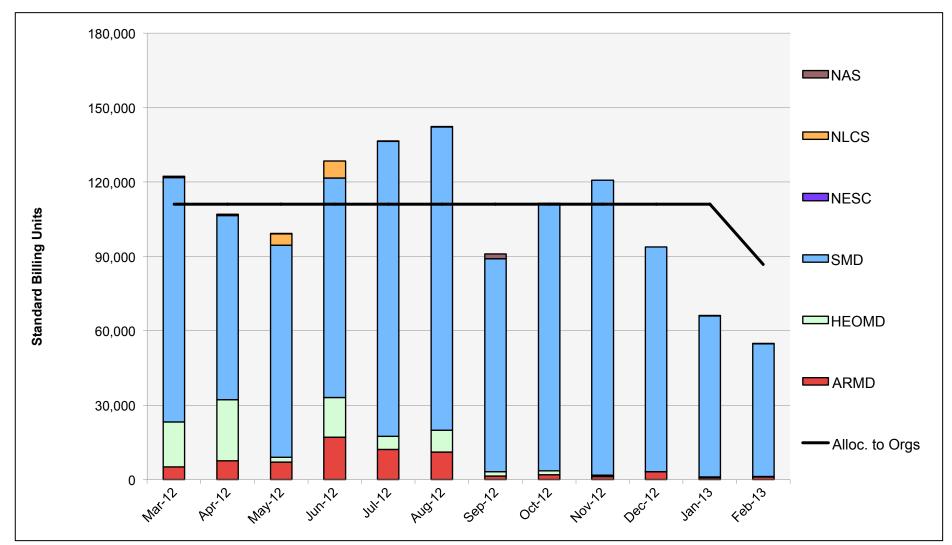
Pleiades: Average Expansion Factor





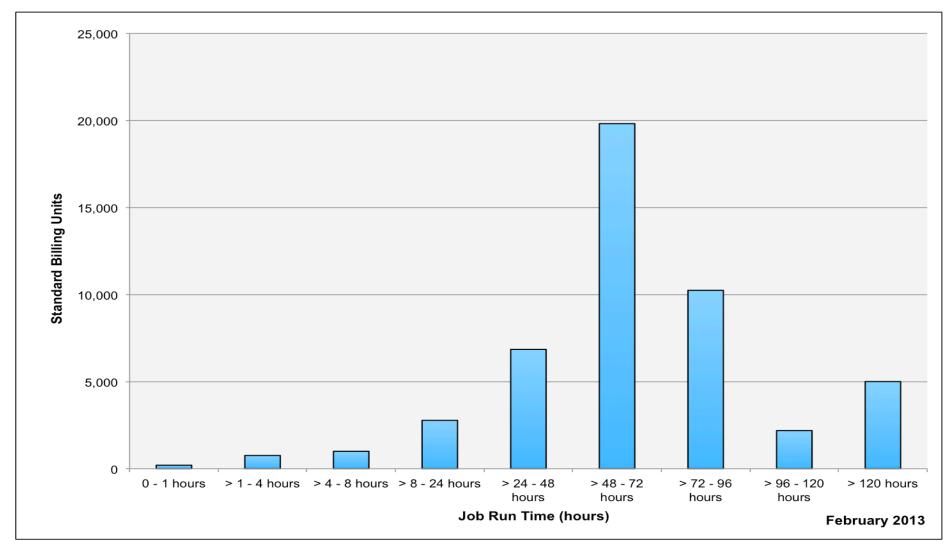
Columbia: SBUs Reported, Normalized to 30-Day Month





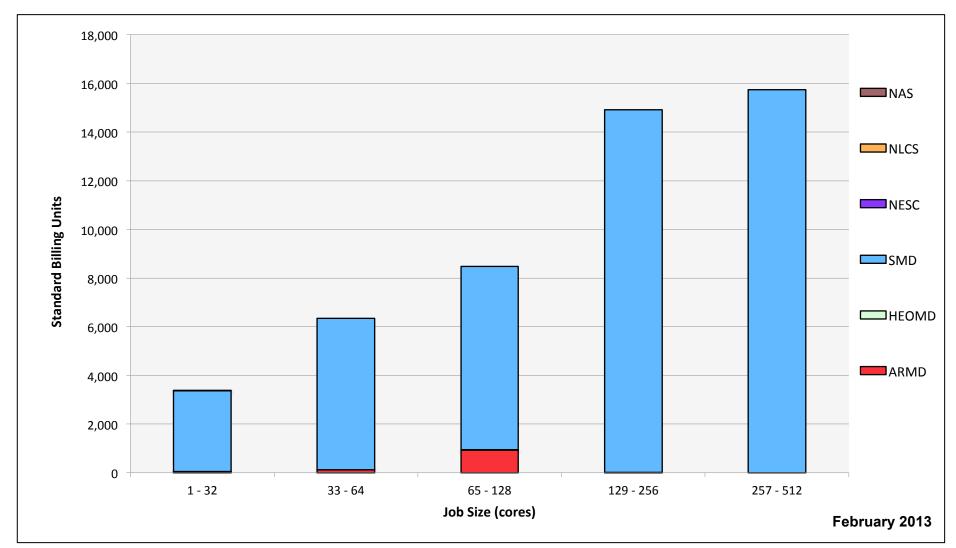
Columbia: SBUs Reported, Normalized to 30-Day Month





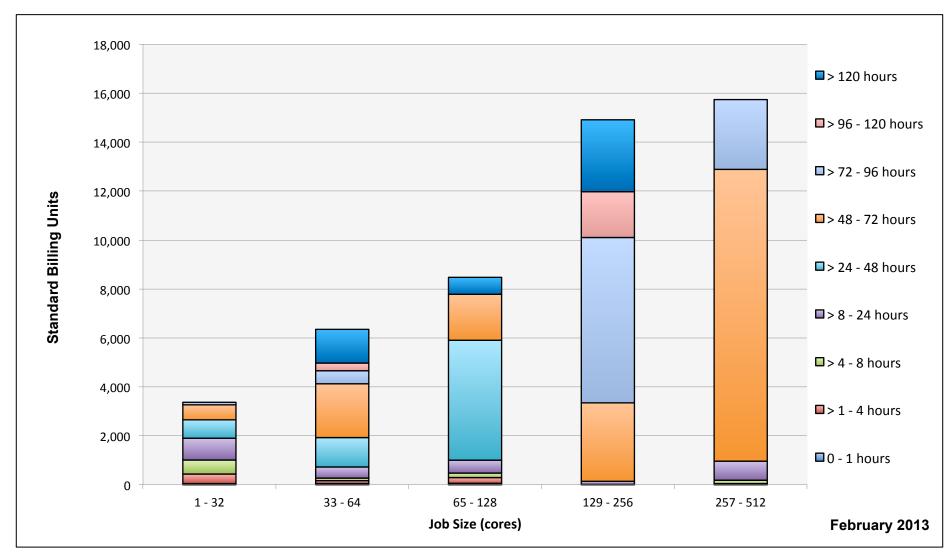
Columbia: Monthly Utilization by Size and Mission





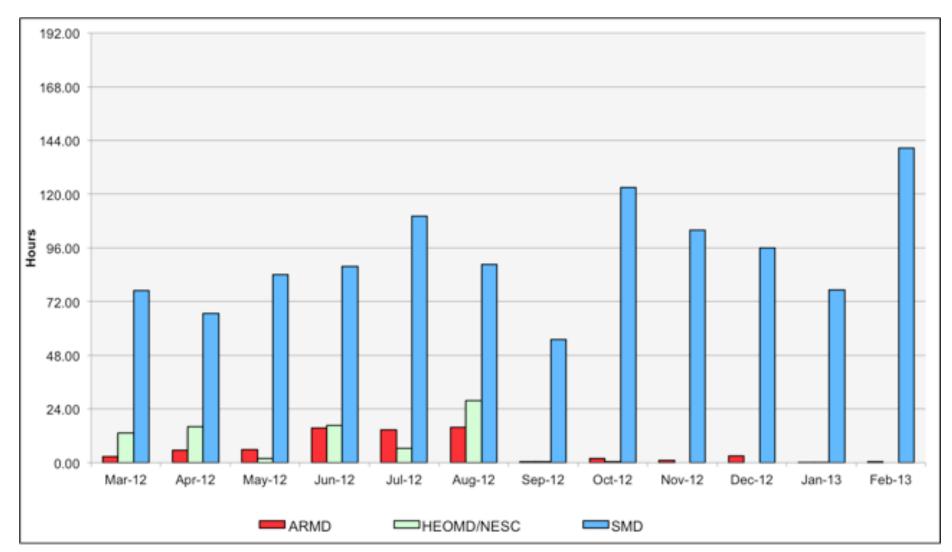
Columbia: Monthly Utilization by Size and Length





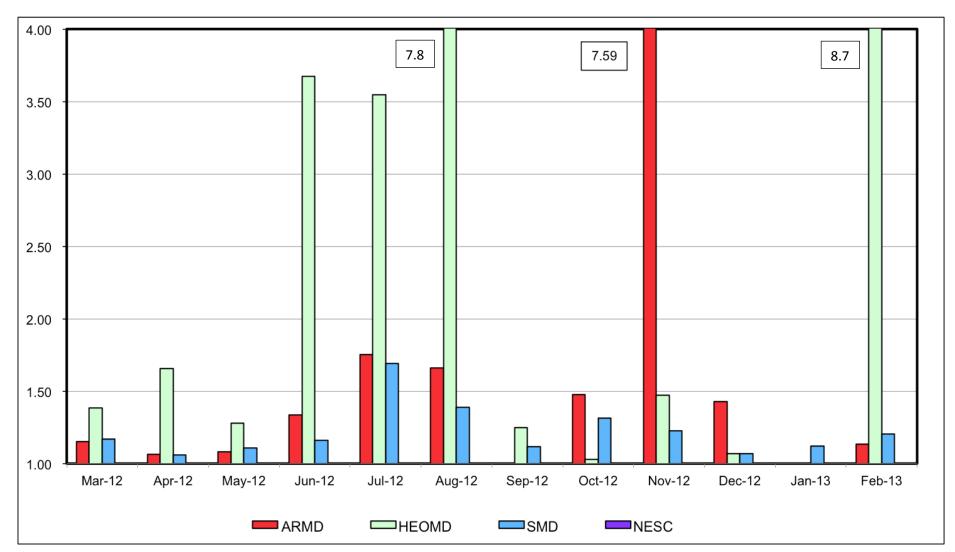
Columbia: Average Time to Clear All Jobs





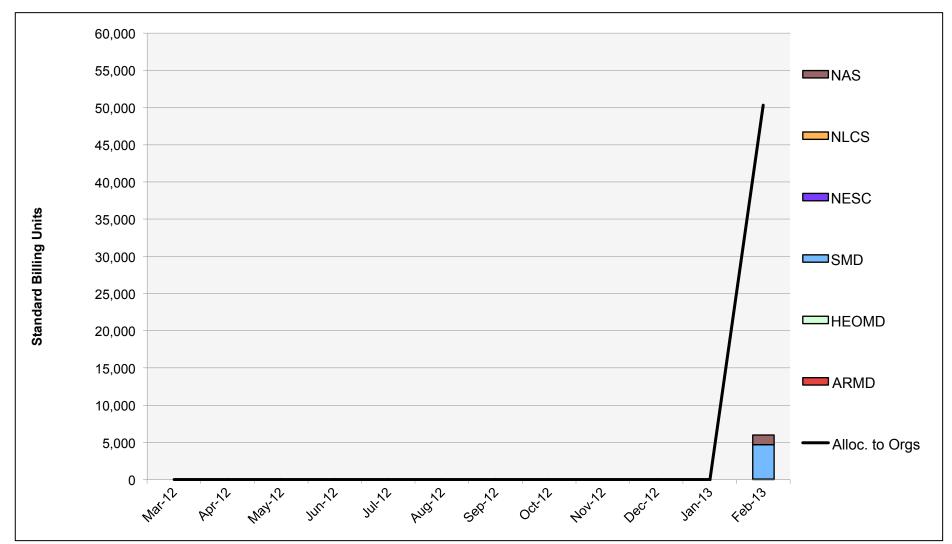
Columbia: Average Expansion Factor





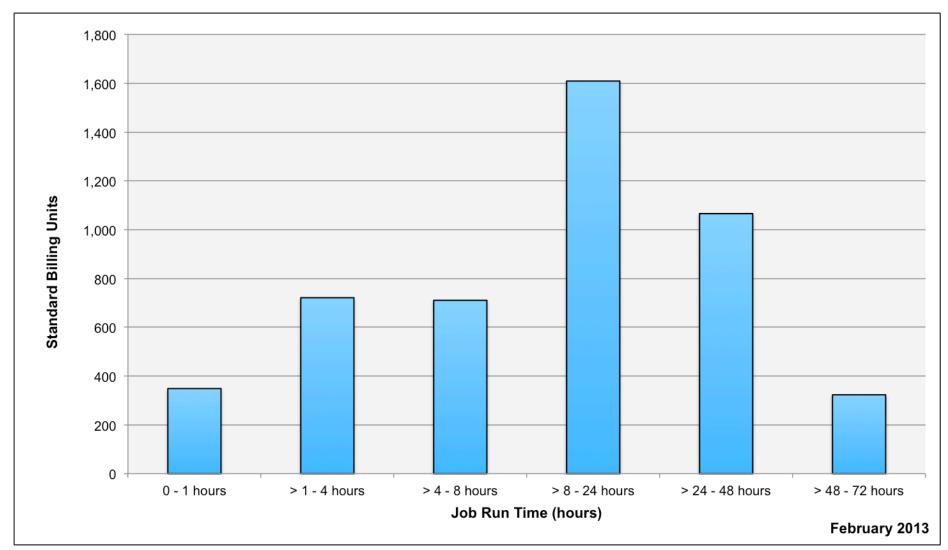
Endeavour: SBUs Reported, Normalized to 30-Day Month





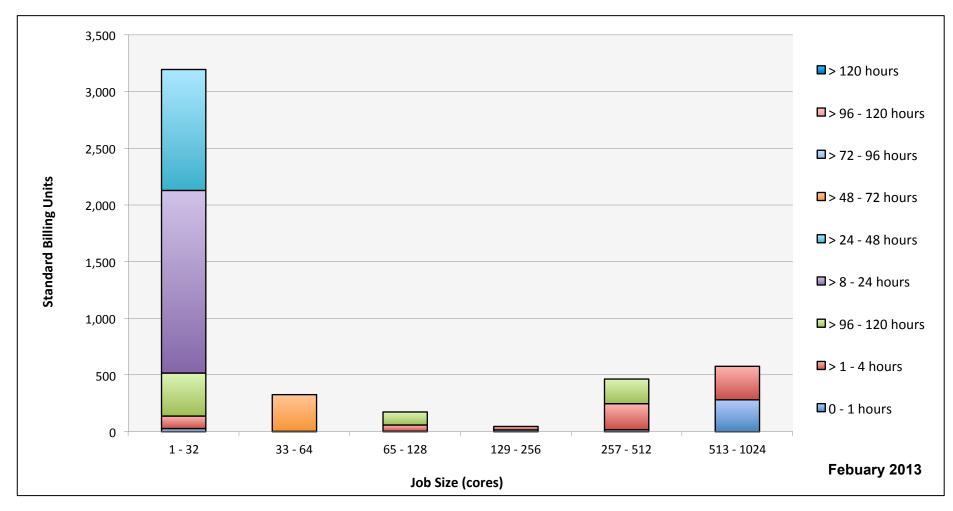
Endeavour: SBUs Reported, Normalized to 30-Day Month





Endeavour: Monthly Utilization by Size and Mission





Endeavour: Monthly Utilization by Size and Length



